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During this year leading researchers and students in numerical algebra and related areas of scientific computation and computer science visited the University of Tennessee and Oak Ridge Laboratory. The theme for the year was the solution of numerical linear algebra problems on computers utilizing new parallel computer architectures. Major highlights included the 10th International Symposium on Numerical Algebra; a workshop on each of the three major research areas in the field: systems of equations, eigenvalue problems, and least squares computations; and a year-long research seminar series.

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Report on the
Special Year on Numerical Linear Algebra
Sponsored by
Departments of Computer Science and Mathematics
University of Tennessee, Knoxville
and
Mathematical Sciences Section,
Engineering Physics and Mathematics Division
Oak Ridge National Laboratory

September 1, 1988

Abstract

The Departments of Computer Science and Mathematics of The University of Tennessee at Knoxville (UTK) and the Mathematical Sciences Section of the Oak Ridge National Laboratory (ORNL) organized a *Numerical Linear Algebra Year* spanning the period from September 1, 1987 to June 30, 1988. During this time, leading researchers in numerical linear algebra and related areas of scientific computation and computer science visited the University and the Laboratory. The activities for the Year were generously supported by the U.S. Air Force Office of Scientific Research, the U.S. Department of Energy, the National Security Agency, the National Science Foundation, and the Science Alliance, a state-supported program at the University of Tennessee. This document is intended to be a report to these agencies, as well as a permanent record of the activities that were supported throughout the year.



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1 Introduction

The Departments of Computer Science and Mathematics of The University of Tennessee at Knoxville (UTK) and the Mathematical Sciences Section of the Oak Ridge National Laboratory (ORNL) organized a *Numerical Linear Algebra Year* spanning the period from September 1, 1987 to June 30, 1988. During this time, leading researchers and students in numerical linear algebra and related areas of scientific computation and computer science visited the University and the Laboratory. The activities for the Year were generously supported by the U.S. Air Force Office of Scientific Research, the U.S. Department of Energy, the National Security Agency, the National Science Foundation, and the Science Alliance, a state-supported program at the University of Tennessee.

It was particularly appropriate for the Special Year to be held at UTK and ORNL. Numerical linear algebra was pioneered at those institutions in the late 1950s when the first large computers became available. One of the pioneers was Alston Householder, formerly a UTK faculty member and head of ORNL's Mathematics Division. Many distinguished mathematicians and computer scientists, such as Wallace Givens and Pete Stewart, joined Householder's staff at ORNL, and leading experts from all over the world, including Jim Wilkinson and Fritz Bauer, were visiting collaborators. The Special Year provided a unique opportunity for many researchers to revisit UTK and ORNL and to remember the experiences of the early years in scientific computing.

The theme throughout the year was on the solution of numerical linear algebra problems on computers utilizing new parallel architectures. The focus was strongly assisted by the availability at UTK/ORNL of a representative computer in each of three major multiprocessor architectural classes - shared memory (Sequent Balance 8000), tightly-coupled distributed memory (Intel iPSC/2 hypercube) and loosely-coupled distributed memory (network of Sun and IBM workstations). In addition, tutorial classes for the long-term visitors were held periodically on how to use these machines.

In addition to the numerous informal and organized discussions that transpired during the year, major highlights included the 10th International Symposium on Numerical Algebra, informally called Gatlinburg X; a workshop on each of the three major research areas in the field - systems of equations, eigenvalue problems, and least squares computations; and a year-long research seminar series. A description of each of these activities is included in this report.

2 Visitors and Local Staff

Several of the visitors (Byers, Pothen, Young) visited on a long-term basis, teaching classes at UT and establishing joint research projects with other UT faculty and ORNL scientists. Other scientists visited for shorter periods.

A list of the visitors follows, along with the dates of their visit.

| | |
|----------------|-----------------|
| Adams, Loyce | 9/14-18/87 |
| Barlow, Jesse | 5/10/88-6/30/88 |
| Beattie, Chris | 1/12-16/88 |
| Björck, Åke | 1/15/88-2/28/88 |
| Bunch, Jim | 3/24-27/88 |
| Byers, Ralph | 1/11/88-3/31/88 |
| Coleman, Tom | 4/18-22/88 |

| | |
|------------------------|---------------------------------|
| Demmel, Jim | 1/10-30/88 |
| Golub, Gene | 11/9-13/87 and 2/8-12/88 |
| Gragg, Bill | 3/28/88-4/1/88 |
| Hansen, Per Christian | 3/1-31/88 |
| Keller-McNulty, Sallie | 5/1-14/88 |
| Kincaid, David | 12/13-20/87 and 1/11-16/88 |
| Klema, Virginia | 3/21/88-4/1/88 |
| LeVeque, Randy | 9/14-18/87 |
| Liu, Joseph | 6/1-24/88 |
| Oleson, Trond | 2/3-5/88 |
| Ortega, Jim | 9/14-18/87 and 10/5-9/87 |
| Paige, Chris | 5/9-20/88 |
| Park, Haesun | 6/13-25/88 |
| Parlett, Beresford | 1/5-20/88 and 5/14-25/88 |
| Peierls, Tim | 1/23-29/88 |
| Plemmons, Bob | 5/1/88-6/30/88 |
| Pothen, Alex | 9/1/87-1/22/88 |
| Saunders, Michael | 10/25/87-11/6/87 and 5/1-21/88 |
| Shoaff, Bill | 3/26/88-4/2/88 and 5/22-28/88 |
| Sorensen, Danny | 1/4-31/88 |
| Stewart, Pete | 3/28/88-4/1/88 |
| Van Loan, Charlie | 5/22-28/88 |
| Warner, Dan | 6/13-16/88 |
| Veselic, K. | 5/14-22/88 |
| Young, David | 9/11/87-12/31/87 and 1/11-16/88 |

Students

Graduate students were invited to participate in the NLA Year. Four students accepted invitations; their names and the dates of their visits are given below:

| | |
|---------------------------------------|------------------|
| Bob Entriken (Stanford University) | 9/27/87-12/31/87 |
| Göran Svensson (Linköping University) | 1/5/88-3/31/88 |
| Bi Roubolo Vona (University of Texas) | 9/11/87-12/31/87 |
| Sheng-you Xiao (University of Texas) | 9/11/87-12/31/87 |

Visitors were asked to submit a brief summary of their activities. The majority of them did so, and their submissions (edited slightly for consistency by Alan George and Bob Ward) are contained in Appendix A. Also included with this report are some of the documents and technical reports that resulted in whole or in part from visitor participation in the program.

Local Support

Faculty and technical staff at UTK and ORNL assisting and participating in the activities for the Special Year were:

| | |
|-------------------------|-----------------------|
| Drake, John (ORNL) | Dunigan, Tom (ORNL) |
| Etheridge, Young (ORNL) | Geist, Al (ORNL) |
| George, Alan (UT/ORNL) | Heath, Michael (ORNL) |

| | |
|---------------------------|-----------------------|
| Karakashian, Ohannes (UT) | Ng, Esmond (ORNL) |
| Ostrouchov, George (ORNL) | Romine, Chuck (ORNL) |
| Serbin, Steve (UT) | Wachspress, Gene (UT) |
| Ward, Bob (ORNL) | Worley, Pat (ORNL) |

A special acknowledgement should go to Mary Drake (UT) and Mitzy Denson (ORNL) who carried the burden of making the innumerable travel and other arrangements for the approximately 40 visitors who participated in the program.

The overall organization and management of the special year was done by Alan George and Bob Ward.

3 10th International Symposium on Numerical Algebra

Fairfield Glade, a scenic location in the Cumberland mountains about 50 miles west of Oak Ridge, was the site of the 10th International Symposium on Numerical Algebra. The symposium was held on October 18-23, 1987 and drew 94 participants with nearly one-third from foreign countries.

The meetings in the series have been informally referred to as the Gatlinburgs despite many changes in location since the first four, which were actually held in Gatlinburg, Tennessee. One of the actions taken at this 10th meeting was to rename the meetings as the Householder Symposia, in honor of Alston S. Householder, founder of the series and organizer of the earliest meetings.

A high point of this year's meeting for many participants was the presence of Householder, who had not been able to attend a "Gatlinburg" since the late 1970s. Householder, now retired and living in Malibu, attended many of the sessions as well as a reception and dinner held in his honor at UTK. He also featured prominently in the reminiscences of Richard S. Varga, banquet speaker at the meeting.

Technical highlights included the presentation on condition number estimation by Nick Higham, the Householder Prize winner; the large number of talks on parallel computation; the different algorithmic approaches to computation on shared-memory and distributed-memory parallel computers; and the large number of informal evening sessions organized by the participants after they arrived at the meeting. The smaller parallel evening sessions, which followed a long day of invited plenary presentations, made the meeting technically intensive.

The next Householder Symposium will be held in Scandinavia in 1990 with Ake Bjorck serving as organizer.

4 Workshops, AMS Meeting

Three workshops were organized for the Special Year on Numerical Linear Algebra. These were held each quarter for five days each. Two lectures of 75-minutes each were presented during the morning sessions, and the afternoon sessions were left open for further discussion or additional topics as requested by participants. Introductory material was provided at each of the workshops so that graduate students and non-experts could also benefit by these workshops.

The first workshop, entitled *A Short Course on the Solution of Sparse Systems of Equations*, was held in the Fall Quarter, 1987. The lecturers, Dr. J. Alan George (UTK and ORNL), Dr. James

M. Ortega (University of Virginia) and Dr. David M. Young (University of Texas at Austin) spoke on the following topics:

George "Sparse Positive Definite Systems: Basic Material"
 "Symbolic Factorization and Data Structures"
 "Elimination Trees and Their Uses"
 "Algorithms for Shared-Memory Parallel Architectures"
 "Algorithms for Local-Memory Parallel Architectures"

Ortega "Parallel Architectures"
 "Jacobi and SOR Methods"
 "Preconditioned Conjugate Gradient Methods"

Young "Iterative Algorithms for the Symmetric Case"
 "Iterative Algorithms for the Unsymmetric Case"

The second workshop, held during the Winter Quarter, was titled *A Short Course on Eigenvalues and Singular Values*. The lecturers were Professor Beresford Parlett (University of California, Berkeley), Professor James Demmel (Courant Institute of Mathematical Sciences, New York), and Dr. Danny Sorensen (Argonne National Laboratory). The titles for their lectures were:

Demmel "Theory and Algorithms for the Dense, Nonsymmetric Eigenproblem"
 "Theory and Algorithms for the Dense, Symmetric Eigenproblem"
 "Condition Numbers and Error Bounds for Eigenvalues and Eigenvectors"
 "A Guided Tour of EISPACK"
 "Recent Research in Parallel Algorithms for the Eigenproblem"

Parlett "Various Eigenvalue Tasks, Error Estimates, Rayleigh-Ritz"
 "Approximations, Subspace Iteration, Lanczos, Arnoldi"
 "Krylov Subspaces and Their Approximation Properties,
 Orthogonality Loss and Paige's Theorem"
 "Implementation Options, Stopping Criteria, Infinite Eigenvalues"
 "The Nonsymmetric Case, Residual Error Bounds"

Sorenson "Divide and Conquer Techniques for Eigenvalue Problems"

The Spring Quarter workshop was titled *A Short Course on Numerical Solution of Least Squares Problems*, and the lecturers were Professor Robert J. Plemmons (North Carolina State University), Dr. Michael T. Heath (ORNL), Dr. George Ostroumov (ORNL), and Dr. Esmond Ng (ORNL). The topics for their lectures were:

| | |
|------------|--|
| Plemmons | "Mathematical Properties" "Numerical Methods" "Constrained Problems and Modified Problems " "Parallel Algorithms " "Some Applications, Including Signal Processing " |
| Heath | "A Structural Approach to Sparse Least Squares Computations" "Variations and Extensions of the Structural Approach to Sparse Least Squares Computations" "A Survey of Other Methods for Sparse Least Squares Computations" |
| Ostrouchov | "Sparse Least Squares Computations in Statistical Applications" |
| Ng | "Software for Sparse Least Squares Computations" |

These workshops were well-attended by UTK faculty and graduate students, ORNL scientists, TVA engineers, and by members of private businesses in the area. Faculty and students from other colleges/universities were also drawn to these workshops.

AMS 841st meeting at Knoxville

Because it was known that this Special Year was being planned, officials of the American Mathematical Society approached the UTK Mathematics Department in January 1987 and suggested that it host a regional meeting of the Society. The Department agreed. The AMS Committee to Select Hour Speakers then asked Professor Alan George to give an hour address and asked that we organize a special session on numerical linear algebra. Professor Jim Bunch of the University of California, San Diego, organized the special session. The meeting was held at the Holiday Inn World's Fair in Knoxville on March 25 and 26. A copy of the program is attached.

5 Seminars

Numerical Linear Algebra Seminars were held on a weekly basis, alternating the location between ORNL and UTK. A listing of these seminars appears below. The announcements and abstracts of each seminar are contained in Appendix B.

| | | |
|------------|----------------------|---|
| Sept. 16 | Randy LeVeque | "Cartesian Grid Methods for Compressible Flow in Irregular Regions" |
| Oct. 5-9 | Workshop | "A Short Course on Numerical Linear Algebra" |
| Oct. 12 | | No seminar (Denver SIAM Meeting) |
| Oct. 19 | | No seminar (Gatlinburg X Meeting) |
| Oct. 26 | Michael Saunders | "Maintaining the Rank of Sparse LU Factors" |
| Nov. 2 | Alan George | "On the Complexity of Sparse LU and QR Factorization of Finite Element Matrices" |
| Nov. 9 | Gene H. Golub | "The Theory of Moments in Linear Algebra" |
| Nov. 16 | Michael Heath | "Parallel Solution of Triangular Systems on Distributed-memory Multiprocessors" |
| Nov. 23 | David M. Young | "Iterative Solution of Partial Differential Equations with Vector and Parallel Computers" |
| Dec. 7 | Alex Pothen | "Computing a Shortest Elimination Tree" |
| Dec. 9 | Linda Hayes | "A Survey of Element-by-Element Techniques for Finite Element Calculations" |
| Dec. 14 | David R. Kincaid | "Software and Numerical Experiments for Nonsymmetric Preconditioned Conjugate Gradient Methods" |
| Dec. 18 | B. Vona & S. Xiao | "Sequent Balance and Hypercube Solutions of Partial Differential Equations" |
| Jan. 11-15 | Workshop | "Short Course on Eigenvalues and Singular Values" |
| Jan. 25 | Tim Peierls | "Sparse Gaussian Elimination in Essential Time" |
| Feb. 1 | Eleanor Chu | "Parallel QR Factorization on a Hypercube Multiprocessor" |
| Feb. 8 | Åke Björck | "Stability Analysis of the Method of Seminormal Equations for Linear Least Squares Problems" |
| Feb. 15 | Holiday | No seminar |
| Feb. 25 | George Ostrouchov | "Sparse Matrix Computations in Analysis of Variance" |
| Feb. 29 | Esmond Ng | "Some Ideas in the Solution of Sparse Linear Least Squares Problems" |
| Mar. 7 | Per Christian Hansen | "Truncated SVD Solutions to Ill-posed Problems With Ill-determined Numerical Rank" |
| Mar. 14 | Ralph Byers | "A Toolbox for Very Special Eigenvalue Problems" |
| Mar. 21 | Eugene Wachspress | "Iterative Solution of Sylvester's Equation" |
| Mar. 28 | Virginia Klema | "Robust Statistics Computations on Parallel Computing Machines" |

| | | |
|---------|-----------------------|--|
| Apr. 11 | Al Geist | "Finding Eigenvalues and Eigenvectors of Unsymmetric Matrices Using A Distributed-memory Multiprocessor" |
| Apr. 18 | Tom Coleman | "Parallel Algorithms for Solving Systems of Nonlinear Equations on a Hypercube Computer" |
| Apr. 19 | Tom Coleman | "On the Convergence Analysis of Algorithms for Constrained Optimization" |
| Apr. 20 | Tom Coleman | "Exploiting Sparsity in Large-Scale Optimization" |
| May 2-6 | Workshop | "Numerical Solution of Least Squares Problems" Holiday Inn at Cedar Bluff |
| May 9 | Sallie Keller-McNulty | "Error-free Sparse Least Squares" |
| May 16 | Bob Plemmons | "Parallel Least Squares Algorithms in Signal Processing" |
| May 23 | No seminar | SIAM Meeting, Madison |
| May 30 | Holiday | No seminar |
| June 6 | Jesse Barlow | "Algorithms for Equality Constrained Least Squares Problems" |
| June 13 | Joseph Liu | "Some Practical Aspects of Elimination Trees in Sparse Factorization" |
| June 20 | Haesun Park | "Jacobi-like Algorithms for the Eigenproblem on a Hypercube" |

A Summary of Activities by Visitor

Loyce Adams

While at Oak Ridge, Dr. Adams was able to discuss the solution of eigenvalue problems (both symmetric and nonsymmetric) with Charles Romine and Al Geist. These discussions led to some ideas that her Ph.D. student, Kevin Gates, is currently pursuing. In fact, Mr. Gates will spend the summer of 1988 at Oak Ridge implementing these ideas on the parallel machines there. David Young and Loyce also had the opportunity to discuss the Fourier analysis of iterative methods. She also participated in discussions with Jim Ortega and the Oak Ridge researchers in parallel computation on the future role of numerical analysis research in the design and use of parallel machines.

Jesse Barlow

Dr. Barlow visited UT and ORNL from May 10 through June 30. During that time he made significant progress on a test code for sparse equality constrained least squares. This test code will eventually result in a technical report that will be submitted for publication.

There was significant progress on his research concerning the interrelation of numerical analysis and computer arithmetic. This work will result in two technical reports that will also be submitted for publication.

Åke Björck

Dr. Åke Björck visited UT/ORNL from Jan. 15–Feb. 14. He has submitted the following abstract of the research which resulted from his participation in the Numerical Linear Algebra Year.

Stabilizing Least Squares Methods by Iterative Refinement

Gaussian elimination with partial pivoting is the standard method for solving unsymmetric, systems of linear equations. However, the stability of this method is only stable when the system is well scaled. Also, for sparse systems, when pivoting requirements have been relaxed the computed solution may be less accurate than the data warrants.

R.D. Skeel has shown that if Gaussian elimination is complemented by iterative refinement the solution is backward stable in the metric of componentwise relative error. This is true even when the refinement uses single precision residuals, and often just a single step of refinement suffices. Moreover, the backward relative error can be computed using the Oettli-Prager bound. Finally the condition number corresponding to this metric can be efficiently estimated using Hager's condition estimator. This technique has recently been pursued for sparse systems by Arioli, Duff and Demmel.

The object of his research has been to apply similar techniques to sparse least squares problems. The benefits are possibly even greater for this class of problems. First, here

the condition number depends strongly on the right hand side. Second, row scaling is not allowed for least squares problems, and the usual condition number has little meaning for "stiff" least squares problems. Also the problem of giving a necessary and sufficient condition for a computed least squares solution to have a small backward error, is still considered to be an open problem.

Most of the theoretical aspects of the research outlined above have been settled. Computational tests are now carried out, and results will be reported in Björck (1989). Some work has also been done in using similar ideas to stably downdate least squares solutions. This work can be found in Björck, Eldén and Waldén (1989).

References:

Björck, Åke (1989), Componentwise backward errors and condition estimates for linear least squares problems. Report LiTH-MAT, to appear.
Björck, Åke, Lars Eldén, and Bertil Waldén (1989), A stable method for downdating a QR decomposition, Report LiTH-MAT, to appear.

James Bunch

Dr. Bunch's participation in the Numerical Linear Algebra Year consisted of organizing and chairing two Special Sessions on Numerical Linear Algebra at the American Mathematical Society Regional Meeting in Knoxville on March 25-26, 1988. Included with this report is a description of the sessions that he prepared for the SIAG/Linear Algebra Newsletter.

Ralph Byers

Dr. Byers' visit to the University of Tennessee and Oak Ridge National Laboratory during the Special Year on Numerical Linear Algebra produced three papers. He expects to have drafts written by September. The abstracts follow.

Numerical Methods for Simultaneous Diagonalization

Jacobi-like methods for simultaneous diagonalization, first suggested for normal matrices by Goldstine and Horwitz in 1959, form a basis for parallelizable numerical methods for structured algebraic eigenvalue problem. We investigate numerical methods for simultaneously diagonalizing pairs of symmetric and pairs of normal matrices. The straight forward "diagonalize one, then diagonalize the other" approach is subject to numerical hazards that may prevent convergence. We introduce a numerically stable, rapidly convergent Jacobi-like algorithm for simultaneously diagonalizing commuting pairs of symmetric matrices. It examines both members of the pair simultaneously. When applied to a pair of non-commuting matrices, the off diagonal sum of squares is minimized, so the algorithm gives a way of measuring the distance from a pair of symmetric matrices to the nearest commuting pair.

Robust Pole Assignment Rescued

Recently, several authors have questioned numerical stability of many pole assignment algorithms including the robust pole assignment methods of Kautsky, Nichols and van Dooren (KNvD). The weak step in the KNvD algorithm is the passage from the selected feasible, eigenvalue-eigenvector pairs to the state feedback matrix. Rounding errors destroy the feasibility of the pairs. This paper describes a numerical method that overcomes infeasible eigenvectors with oblique projections onto feasibility. The resulting closed loop system matrix is within a rounding-error-small relative perturbation of a matrix with the desired eigenvalues. Well-conditioned systems eigenvectors are also assigned to full accuracy, but ill-conditioned systems may not be.

On Distance to Uncontrollability

A pair of matrices (A, B) , is controllable if no left eigenvector of A lies in the left null space of B . Controllability is a kind of nonsingularity requirement for many problems in linear control theory. In a preliminary study of a partly heuristic method for measuring the distance from a controllable pair to the nearest uncontrollable pair Jim Demmel and Bo Kagstrom discovered that nearly uncontrollable systems do occasionally occur in practice. Examples they cited included an aircraft control system a nuclear rocket engine control system and an automobile engine control system. Remedies may be as easy as modifying a mathematical model, however, there is a need for a practical, reliable test for near uncontrollability. Using a quadratically convergent variation of the Byers bisection algorithm, the problem of finding the nearest uncontrollable pair reduces to a one dimension algorithm.

In addition, Ralph attended the AMS Regional Meeting at Knoxville, March 25-26, 1988, where he gave a talk titled "A Toolbox for Very Special Eigenvalue Problems". It included some material from the first abstract.

Tom Coleman

Dr. Coleman's short visit did not directly result in a research report or article. However, the paper "Solution of Nonlinear Least Squares Problems on a Multiprocessor" did benefit from discussions at ORNL. This paper is co-authored by Paul E. Plassman. It is not yet a technical report nor have they submitted the paper to a journal. They expect to do both shortly.

Jim Demmel

Dr. Demmel's activities over the last year may be divided into four areas, all of which benefited from his visit during the Numerical Linear Algebra Year at ORNL/UTK. These areas are: A new, more accurate SVD algorithm, Solving sparse linear systems with sparse backward error, A block, nonsymmetric QR algorithm for parallel and vector machines, and LAPACK - a portable, parallel numerical linear algebra library.

A new, more accurate SVD algorithm. This is joint work with W. Kahan at the University of California at Berkeley. Computing the singular values of a bidiagonal matrix is the final phase of the

standard algorithm for the singular value decomposition of a general matrix. They present a new algorithm which computes all the singular values of a bidiagonal matrix to high relative accuracy independent of their magnitudes. In contrast, the standard algorithm for bidiagonal matrices may compute small singular values with no relative accuracy at all. Numerical experiments show that the new algorithm is comparable in speed to the standard algorithm, and frequently faster. They also show how to accurately compute tiny eigenvalues of some classes of symmetric tridiagonal matrices using the same technique.

Solving sparse linear systems with sparse backward error. This is joint work with I. Duff and M. Arioli of Harwell Laboratory. When solving sparse linear systems, it is desirable to produce the solution of a nearby sparse problem with the same sparsity structure. This kind of backward stability helps guarantee, for example, that one has solved a problem with the same physical connectivity as the original problem. Theorems of Oettli, Prager and Skeel show that one step of iterative refinement, even with single precision accumulation of residuals, guarantees such a small backward error if the original matrix is not too ill-conditioned and the solution components do not vary too much in magnitude. We incorporate these results into the stopping criterion of an iterative sparse matrix solver and verify by numerical experiments that the algorithm almost always stops after one step of iterative refinement with a componentwise relative backward error at the level of machine precision. Furthermore, this stopping criterion is very inexpensive. We also discuss a condition estimator corresponding to this new backward error which provides an error estimate for the computed solution. This error estimate is generally tighter than estimates provided by standard condition estimators. We also consider the effects of using a drop tolerance during the LU decomposition. Additional insights were gained through conversations with David Young during the short course on eigenvalue problems, held as part of the Numerical Linear Algebra Year. In particular, they discussed the issue of whether the backward error should be attributed to the right hand side vector or the matrix; Young pointed out that if all the error is attributed to the right hand side sparsity is trivially maintained, but at the cost of loss of sparsity in the right hand side.

A block, nonsymmetric QR algorithm for parallel and vector machines. This is joint work with Z. Bai at the Courant Institute. The usual QR algorithm for finding the eigenvalues of a Hessenberg matrix H is based on vector-vector operations, e.g. adding a multiple of one row to another. The opportunities for parallelism in such an algorithm are limited. Based on work of C. C. Paige, we have reorganized the work of QR to permit either matrix-vector or matrix-matrix operations to be performed, both of which yield more efficient implementations on vector and parallel machines. The idea is to chase a k -by- k bulge rather than a 1-by-1 or 2-by-2 bulge as in the standard algorithm. They will report their preliminary numerical experiments on the CONVEX C-1 vector machine. This work benefited greatly from collaboration with B. Parlett who also visited during the short course on eigenvalue problems, held as part of the Numerical Linear Algebra Year. In particular, we were able to identify the computational core of Paige's ideas which led to the new algorithm.

LAPACK - a portable, parallel numerical linear algebra library. This is joint work with J. Dongarra, D. Sorensen and C. Bischof of Argonne National Lab, A. Greenbaum and Z. Bai of the Courant Institute, and J. Du Croz and S. Hammarling of the Numerical Algorithms Group, Ltd. LAPACK is a library of portable, high-performance linear algebra subroutines being designed for use on supercomputers and shared-memory parallel processors, and covering most of the facilities offered by EISPACK and LINPACK. High-performance and portability will be achieved by constructing the library from the Level 3 BLAS, a set of Basic Linear Algebra Subroutines for matrix-matrix

operations. The library will also include recently devised parallel divide and conquer algorithms for the symmetric eigenproblem and SVD. All the previously mentioned work in this report will appear in LAPACK, and so benefited from the visit during Numerical Linear Algebra Year. In particular, Danny Sorensen and Jim Demmel outlined the main section of a document describing the LAPACK algorithms for the symmetric eigenproblem.

Bob Entriken

From September till December of 1987, Bob Entriken visited the Oak Ridge National Laboratory. His first four weeks were spent in seminars and at the Gatlinburg Conference at Fairfield Glade, TN. The first seminar series was a one-week short course in the use of their Sequent and Hypercube parallel computers given by Chuck Romine and Tom Dunigan and was held at The Oak Ridge Associated Universities. The second week he spent at The University of Tennessee attending a one-week seminar series on Numerical Linear Algebra given by Alan George, Jim Ortega and David Young. During most of the next two weeks the Gatlinburg Conference took place.

Following this strong introduction into the world of Numerical Linear Algebra, Bob set about working on the Sequent computer. In the following two months he designed and implemented a preliminary version of Parallel Decomposition of Staircase Linear Programs. Building on work done previously at Stanford which involved the Serial Decomposition of Staircase Linear Programs, Bob designed the new software by incorporating what he had recently learned and previous ideas. At the completion of his stay at Oak Ridge, Bob had successfully demonstrated the new parallel algorithm in principle and isolated several key measures of performance. Finally, he presented these preliminary results in a one-hour presentation and prepared an ORNL technical report on this material called "The Parallel Decomposition of Linear Programs".

Gene Golub

Prof. Golub paid two visits to ORNL/UTK during the special year. In addition to research discussions with the staff and visitors, he performed two special tasks for UTK and ORNL. He enjoyed the honour of presenting the first Robert T. Gregory Memorial Lecture at the University of Tennessee on November 11, 1987. The title of his talk was "The Jacobi Method, Bob Gregory and Recent Developments." For several days during his second visit, he participated as a member of the Advisory Committee for ORNL's Engineering Physics and Mathematics Division. The division held an Information Meeting for the committee and other interested guests with administrative overviews, technical talks and informal discussions.

Bill Gragg

Dr. Gragg, during his four-day visit to ORNL, worked on several aspects of algorithms related with positive definite Toeplitz matrices and unitary Hessenberg eigenproblems, and inverse eigenproblems. Several papers, with his co-authors Gregory Ammar, and Lothar Reichel, are now in final form, and will appear in various journals. Some of these are:

Gragg and Ammar, *Constructing a Unitary Hessenberg matrix from Spectral Data* (Presented at NATO Advanced Study Institute on Numerical Linear Algebra, Digital Signal Processing, and Parallel Algorithms, Leuven, Belgium, August 1988).

Gragg and Ammar, *A Note on an Inverse Eigenproblem for Band Matrices*.

Gragg and Reichel, *A Divide and Conquer Method for Unitary and Orthogonal Eigenproblems*.
(To be submitted to *Numerische Mathematik*.)

Per Christian Hansen

During the month of March Per Christian Hansen visited the University and the Laboratory to work on techniques for numerically solving ill-posed linear least squares problems. He finished two reports, one describing the use of truncated singular value decompositions and the other of truncated generalized singular value decompositions. The abstracts are given below, and copies of the articles are included with this report.

Solution of Ill-Posed Problems by Means of Truncated SVD

We investigate Truncated SVD (TSVD) solutions to ill-posed least squares problems involving matrices with ill-determined as well as well-determined numerical rank. If a discrete Picard condition is satisfied, then in both cases the truncation parameter can be chosen such that the TSVD solution is satisfactory. The appropriate truncation parameter, giving the optimal signal-to-noise ratio in the solution, is the minimizer of the generalized cross-validation function.

Regularization, GSVD and Truncated GSVD

The generalized SVD (GSVD) is used to analyze two alternative methods for solving ill-posed problems: regularization in general form, and truncated SVD. We give conditions in which suitable solutions can be found, discuss the perturbation theory, and show that the optimum regularization and truncation parameters can be computed via generalized cross-validation. Our analysis also sheds light on a particular method, based on a transformation to standard form, that avoids the numerical difficulties associated with computation of the GSVD.

Sallie Keller-McNulty

Dr. Keller-McNulty's two-week visit resulted in the completion of a joint research project with Dr. George Ostroumov of ORNL. The abstract of the resulting paper is given below.

Error-Free Least Squares Based on LU Factorization Applicable to Sparse Problems

A numerical method that allows error-free computation of least squares solutions to sparse linear systems of equations is developed. This method requires the sparse linear systems of equations to have rational entries. To avoid error that is inherent in floating-point arithmetic, multiple modulus residue arithmetic is applied to a modified version of the LU decomposition with back-substitution.

David Kincaid

Dr. David R. Kincaid of The University of Texas at Austin visited Oak Ridge National Laboratory (ORNL) and the University of Tennessee (UT) during the week of December 3–19, 1987. While at ORNL, he gave a talk entitled “Software and Numerical Experiments for Nonsymmetric Preconditioned Conjugate Gradient Methods.” At both ORNL and UT, he consulted with others, discussed his current research, and attended seminars.

The following report resulted, in part, from his participation in the UT/ORNL Numerical Linear Algebra Year: “NSPCG User’s Guide, Version 1.0: A Package for Solving Large Sparse Linear Systems by Various Iterative Methods,” Thomas C. Oppe, Wayne D. Joubert, David R. Kincaid, Report CNA-216, Center for Numerical Analysis, The University of Texas at Austin, April 1988.

Dr. David R. Kincaid returned to Knoxville, with Dr. David M. Young, to attend the short course “Matrix Eigenvalues and Singular Values” which was held January 11–15, 1988. The lectures were given by Drs. Beresford Parlett, James Demmel, and Danny Sorensen.

Randy LeVeque

While visiting Oak Ridge Dr. LeVeque gave a talk on his work on “Cartesian grid methods for flow in irregular regions”, describing one way to derive boundary conditions for finite volume methods on regular Cartesian grids which are cut by irregular boundaries. He discussed some of his work on partial differential equations and computational fluid dynamics with several of the ORNL staff with interests in this area, and had learned of some very interesting problems in this direction.

On the linear algebra side, Dr. LeVeque discussed some joint work on Fourier analysis of the SOR method with his coauthors Loyce Adams and David Young, who were also visiting Oak Ridge.

Joseph W.H. Liu

A seminar was given at the Oak Ridge National Laboratory on June 13, 1988. The title of the talk was “Some practical aspects of elimination trees in sparse factorization”.

During the visit of almost a month, Dr. Liu studied the various distributed algorithms for solving triangular linear systems [1,2,3,4,5,6]. His motivation was to see how such ideas can be applied to solving triangular systems involving large sparse Cholesky factor matrices. In particular, he considered the use of the basic cyclic schemes by Chamberlain [1] and Li and Coleman [4]. These cyclic schemes assume a wrap mapping of columns of the triangular matrix onto the multiprocessors.

To adapt the cyclic schemes for sparse triangular factors, it is required to generalize the algorithm to handle general mappings. As a result of the investigation, a report “A note on cyclic algorithms for distributed triangular solution”, was written. The generalized cyclic schemes make use of the notion of variable segment sizes. The abstract of the report is as follows.

A Note of Cyclic Algorithms for Distributed Triangular Solution

The cyclic vector-sum algorithm by Li and Coleman solves triangular systems on distributed-memory multiprocessors. It assumes a wrap mapping of columns of the triangular matrix onto the multiprocessors. In this note, we generalize the algorithm to handle general mappings. The generalization will be useful when the mapping is inherited from a previous computational phase (such as factorization), or when the algorithm is adapted to solve sparse triangular systems.

- [1] R. M. Chamberlain, "An algorithm for LU factorization with partial pivoting on the hypercube", Tech Report CCS 86/11, Chr. Michelson Institute.
- [2] S. C. Eisenstat, M. T. Heath, C. S. Henkel, and C. H. Romine, "Modified cyclic algorithms for solving triangular systems on distributed-memory multiprocessors," SISSC, vol. 9, pp. 589-600, 1988.
- [3] M. T. Heath and C. H. Romine, "Parallel solution of triangular systems on distributed-memory multiprocessors," SISSC, vol. 9, pp. 558-588, 1988.
- [4] G. Li and T. F. Coleman, "A new method for solving triangular systems on distributed memory message-passing multiprocessors", Tech. Report TR 87-812, DCS, Cornell University, Ithaca, New York, 1987.
- [5] G. Li and T. F. Coleman, "A parallel triangular solver for a distributed-memory multiprocessor," SISSC, vol. 9, pp. 485-502, 1988.
- [6] C. H. Romine and J. M. Ortega, "Parallel solution of triangular systems of equations," Parallel Computing, vol. 6, pp. 109-114, 1988.

James Ortega

Dr. Ortega was one of the three lecturers at the Linear Equation Short Course in October. No publications resulted from this activity; however, many active discussions were held with local staff and visitors on current research and design issues in parallel computing.

Haesun Park

Haesun Park continued her research on Jacobi-like algorithms for eigenvalue problems with Patricia Eberlein, of SUNY Buffalo. This study has been directed toward implementing these algorithms on the hypercube. They discovered some new Jacobi orderings for parallel implementation of the Jacobi-like algorithms on a ring-connected array of processors. These orderings are optimal in that they require a minimum number of stages with minimal message passing to complete each sweep. To handle oversized problems, when the matrix order does not fit the number of available processors, Park studied block column schemes. In addition, research was carried out on the convergence behavior of Jacobi-like algorithms for the non-symmetric eigenvalue problem. For all of the above studies, implementations were done on the Intel iPSC2 hypercube for analyzing performance behavior.

Beresford Parlett

Most of Dr. Parlett's time was taken up with the lectures for the short course on "Eigenvalues and Singular Values" held in January. No reports were directly connected to his brief visit.

However he has worked intensively on five problems in NLA this year. Discussions were held with many of the staff and visitors on these topics.

1. The forward instability of tridiagonal QR. A student has just filed his thesis. It will be an interesting report.
2. Lanczos using an improper inner product. Beresford was able to discuss this with Kresimir Veselić during his visit.
3. $\exp(Bt)$ via Schur form for real B . This long drawn out project is essentially complete. Another Ph.D. student should produce documentation this summer.
4. How to swap diagonal blocks in the Schur form. He is waiting for an ex-student to write up what they have done.
5. Misconvergence in symmetric Lanczos. Accepted for the NPL Wilkinson Proceedings. A technical report is out.

Tim Peierls

Tim Peierls worked on his Cornell Ph.D. thesis, entitled "Algorithms for Sparse Gaussian Elimination with Pivoting," and also gave a talk on a paper he co-authored with John Gilbert, entitled "Sparse Partial Pivoting in Time Proportional to Arithmetic Operations," which is scheduled for publication in SISSC in September. Considerable interactions and collaborative discussions on his thesis topic were held with Esmond Ng at ORNL.

Robert J. Plemmons

One month, May 1-31, 1988, was spent visiting the University of Tennessee at Knoxville and the Oak Ridge National Laboratory. During this time the following activities took place.

1. A series of 5 lectures were given at the NLA Spring Workshop on Least Squares Problems. An outline of these tutorial and survey lectures given May 2-6, 1988, follows.

Schedule of Tutorial Lectures

- (a) Monday May 2: Mathematical Properties of LS
 - Introduction
 - Characterizations
 - Pseudoinverses and Rank Deficient Problems

- Sensitivity Bounds
- Survey of Application Areas

(b) Tuesday May 3: Numerical Methods for LS

- Normal Equations
- Orthogonal Methods
- Singular Value Decomposition
- Rank Deficient Computations
- Iterative Methods

(c) Wednesday May 4: Constrained & Modified LS

- Equality & Inequality Constraints
- Updating & Downdating Modifications

(d) Thursday May 5: Parallel Algorithms for LS

- Survey of Orthogonal Factorization Schemes
- Structured Forms
- Inverse Factorizations
- Modifications

(e) Friday May 6: Some Engineering Applications

- Geodetic Surveying and Photogrammetry
- Structural Analysis and Design
- Signal Processing

2. A seminar lecture on his recent research on certain numerical linear algebra problems in signal processing was given on May 16. An abstract follows.

*Parallel Algorithms for Least Squares Filtering
in Signal Processing*

We are concerned with the investigation of parallel algorithms for least squares modifications in signal processing. The first part of the talk involves a comparison of various algorithms for least squares updating and downdating on the hypercube, including comparisons of Givens rotations and Householder transformations for multiple updates. Computational tests on an iPSC hypercube are discussed. This part includes joint work with D. Agrawal, C. Henkel, and S. Kim at NCSU and with M. Heath at ORNL. The second part of the talk involves parallel least squares modifications using inverse factorizations. The process of modifying least squares computations by updating the covariance matrix has been used in control and signal processing for some time in the context of linear sequential filtering. Here we give an alternative derivation of the process and provide extensions to downdating. Our purpose is to develop algorithms that are amenable to implementation on modern multiprocessor architectures. We have attempted to provide some new insights into least squares modification processes and to suggest parallel algorithms for implementing Kalman type sequential filters in the analysis and solution of estimation problems in control and signal processing. This part of the presentation is joint with C. Pan at NIU.

3. A paper titled *Recursive Least Squares Computations on a Hypercube Multiprocessor Using the Covariance Factorization* was written with co-author Charles S. Henkel as part of the Year of Numerical Linear Algebra activities. The paper will be submitted to the SIAM J. on Scientific and Statistical Computing.

Alex Pothen

Two papers, whose titles are given below, resulted from Dr. Pothen's visit to UTK/ORNL. In addition, collaborative research was initiated with Chuck Romine of ORNL and future publications are expected.

Pothen, Alex. *Simplicial Cliques, Shortest Elimination Trees, and Supernodes in Sparse Cholesky Factorization*. CS-88-13. Dept. of Computer Science, The Pennsylvania State University, University Park, PA 16802. April 1988. Submitted to LAA.

Pothen, Alex. *The Complexity of Optimal Elimination Trees*. CS-88-16. Dept. of Computer Science, The Pennsylvania State University, University Park, PA 16802. April 1988.

Michael Saunders

Dr. Saunders visited the University of Tennessee and Oak Ridge National Laboratory for two weeks in October 1987 and for three weeks in May 1988, as a participant in the Special NLA Year.

For much of the time he pursued development of the sparse matrix package LUSOL described in the following reference:

P. E. Gill, W. Murray, M. A. Saunders and M. H. Wright (1986). Maintaining *LU* factors of a general sparse matrix, *Linear Algebra and its Applications* 88/89, pp. 239-270.

During his visit, he was able to complete most of the planned implementation changes. (These enable the package to handle singular matrices better than before, by maintaining the *U* factor of upper-trapezoidal form.) Michael also gave a seminar on the proposed modifications during his first visit, and received some valuable suggestions as a result. He is testing the modified package and working on the preparation of a new user's manual. The manual will eventually appear, and support from the Special NLA Year will be gratefully acknowledged.

One of his students, Robert Entriken, was a visitor during the autumn quarter, and without question his doctoral research profited enormously from the occasion—particularly from the exposure to parallel computing.

Bill Shoaff

A brief description of the work which resulted from his participation in the UT/ORNL Special Year in Numerical Linear Algebra is included with this report. Although this work is still incomplete, the experience at Oak Ridge was essential to the initiation of this research.

Danny Sorensen

Dr. Sorensen visited ORNL and UT during the month of January, 1988 as a participant in the Special Year in Numerical Linear Algebra. Following is a brief summary of his activities during this period.

1. Participated in a Short Course on Eigenvalues during the week of January 12-16. Contributed to the lectures by giving a talk on divide and conquer techniques for the symmetric eigenvalue problem and the singular value decomposition.
2. Prepared the paper "A Divide and Conquer Algorithm for Computing the Singular Value Decomposition" (jointly authored with E. R. Jessup) for publication in the proceedings of the Third SIAM Meeting on Parallel Processing for Scientific Computing that was held at Los Angeles, CA, in December, 1987.
3. Prepared a working plan for the portion of LAPACK that will be concerned with the symmetric eigenvalue problem and the singular value decomposition. This was done in collaboration with Jim Demmel. The opportunity to interact with Jim during this period was very timely and fruitful.
4. Visited Virginia Polytechnic Institute at Blacksburg, VA, and gave a talk on parallel algorithms for eigenvalue problems. He was able to continue interaction with Chris Beattie that was initiated during the eigenvalue workshop at UT.
5. Studied several research problems. Most of these efforts were concerned with finding a way to selectively introduce small subdiagonal elements to a matrix in Hessenberg form using orthogonal similarity transformations. Three approaches have been investigated. Two of these (rank one tearing, iterative "bulge chasing") have been found to be unworkable. A third technique involving partial reduction to Hessenberg form followed by an iteration to find a reducing subspace is still being considered.

Pete Stewart

Dr. Pete Stewart took the opportunity to work on his paper entitled, "JEEP A Customization of the L^AT_EX Article and Report Styles". This was not directly related to the Special Year in NLA, nevertheless it is a valuable tool which can be used and appreciated by all.

Göran Svensson

During his stay in Tennessee Göran worked with development of a Block-Hestenes method for computation of the SVD. He implemented it on the Intel Hypercube at ORNL and was able to do some testing of it. He has not yet written any paper about it, but has since talked on the subject at the Nordic Section of SIAM Meeting in Bergen, Norway. Following is an abstract of this talk:

**A Block-Hestenes Method
for Computing the SVD on a Hypercube**

Hestenes' method is a one-sided Jacobi method for computation of the singular value decomposition of a matrix A. A is transformed into a matrix with orthogonal columns (or rows), by means of orthogonal rotations. In a block-Hestenes process A is divided into column blocks, and the blocks are rotated pairwise, following some predetermined scheme so that all blocks are orthogonalized against each other. When all columns are orthogonal, they are normalized, and the norms are the singular values. This method is well suited for use on a parallel computer, because orthogonalizations of different blocks are independent, and could be carried out at the same time. In this implementation a hypercube architecture is used. The blocks are sent to the processors, where they are orthogonalized, and then they are moved between the processors, using only closest-neighbour communication, before the next orthogonalization.

Kresimir Veselić

Dr. Veselić wrote a paper entitled, "A Note on One-sided Diagonalization Algorithms", during his visit to UTK. The paper is attached. In addition, collaborative discussions were held with Beresford Parlett on algorithms for generalized eigenvalue problems.

Bi Roubolo Vona

During the fall semester of 1987, Bi Roubolo Vona participated in the Special Year of Numerical Linear Algebra as a member of a team from the Center for Numerical Analysis at The University of Texas at Austin.

The group was composed of the supervising professor David M. Young, his colleague Mr. Xiao Shengyou, and Mr. Vona. Dr. David Kincaid joined them for a week in December.

While in Tennessee, Mr. Vona worked as a graduate research assistant appointed half-time by The University of Texas at Austin, and part-time by The University of Tennessee at Knoxville.

He was primarily concerned with learning how to use the Sequent Balance and the Hypercube. After attending a short course on parallel programming he did some experiments on the parallel implementation of iterative techniques on the Intel iPSC Hypercube and the Sequent Balance 8000 at ORNL. A substantial amount of his time was also devoted to various seminars and other courses on vector and parallel methods in numerical linear algebra, both at UTK and ORNL.

Mr. Vona attended the short courses on Parallel Programming and the Solution of Sparse Systems of Equations, and the 1987 Gatlinburg Conference.

Specific projects that he worked on were:

1. Project on The Hypercube and The Sequent Balance at ORNL.

Parallel iterative solutions of a two-dimensional elliptic partial differential equation of the form

$$Au_{xx} + CU_{yy} + DU_x + EU_y + FU = G$$

in the unit square with Dirichlet boundary conditions.

The problem lends itself to the decomposition by a rectangular grid of computational processes for the solution on the Hypercube and the Sequent Balance. Some performance studies were made for various methods such as the Jacobi-Chebyshev, the Jacobi-conjugate gradient, and the Multicolor-Sor with different computational grid dimensions.

The results will be compiled as a research report for the Center for Numerical Analysis at The University of Texas at Austin.

2. Project with Dr. Eugene Wachspress.

See "Preconditioners for Matrices Which Have Full Coupling of The Boundary Nodes" manuscript by Eugene Wachspress, December 1987.

3. Ongoing work.

"High-level" parallel iterative methods for the solution of sparse linear systems.

These methods are described in a recent paper (manuscript) by David M. Young, entitled "The Search for High-level Parallelism for the Iterative Solution of Large Sparse Linear Systems." They are currently focussing on two methods:

(a) The Spectral Decomposition Method for the solution of the system

(i) $Au = b$

when the smallest and the largest eigenvalues of the SPD matrix A are known.

(b) The Method of Rational Iterations for the system (i) and also for the related system of ordinary differential equations

(ii) $du/dt = -Au + b$.

Shengyou Xiao

From September 1, 1987, to December 20, 1987, Shengyou visited the University of Tennessee at Knoxville and the Oak Ridge National Laboratory along with his supervisor Professor David M. Young.

During his stay Shengyou attended several intensive short courses and seminars, which were very closely related to the recent research in numerical linear algebra. In particular, he attended the short course on the solution of large sparse systems of linear equations, given by Professor James M. Ortega, Professor David M. Young, and Professor J. Alan George. The other short course that he attended was the parallel computing course given by Dr. M. T. Heath, Dr. Tom Dunigan and Dr. Chuck Romine. In this course, a general introduction to currently existing parallel computer systems was presented. The focus of the course was on two popular machines: Sequent balance 8000/21000 which is a shared-memory system, and Intel iPSC which is a distributed-memory

system. The parallel library routines and facilities of these two systems were discussed. Also some of their computing experience was given.

In addition to attending the seminars, he also conducted some experiments in solving simple partial differential equations on parallel computers, using iterative methods for the resulting discrete linear system. The experiments focused on the performance of different methods in terms of execution time, speedup, communication time, storage, synchronization, etc. Several common problems in parallel computing had been considered, such as various local and global communication schemes (on distributed memory machine) and their effect on the efficiency of the particular parallel algorithm, domain decomposition for parallelism, and the adaptation of a serial code to a parallel environment shared-memory and distributed memory machine.

David Young

Dr. Young spent the Fall Semester in Knoxville, Tennessee, where he was a Visiting Professor in the Department of Mathematics at the University of Tennessee (UTK) and a Visiting Scientist in the Mathematical Sciences Section of the Oak Ridge National Laboratory (ORNL). His visit to Tennessee was made in connection with the Special Year in Numerical Linear Algebra.

One of the main objectives of David's visit was to learn as much as possible about parallel computers so this knowledge could be applied to his research on numerical methods for solving partial differential equations. As a step toward this objective, David and two of his students attended a short course on parallel computers which was given at Oak Ridge. Following this, test problems were run on the Sequent Balance and on the Hypercube computers. He participated in discussions with staff members at ORNL and at UTK as well as visitors on the use of parallel processors. He also attended a number of seminars at both locations. In addition he was able to attend several conferences and participated in several short courses.

His activities included work in the Mathematical Sciences Section at ORNL and at the Department of Mathematics at the University of Tennessee. David noted that he was provided with excellent office facilities in each place as well as ready access to computing equipment.

David also felt that an important aspect of the program was the opportunity to interact with researchers in his field. Listed below are some of the researchers with whom he interacted.

| Oak Ridge | UTK | Visitors |
|----------------|-------------------|------------------|
| Bob Ward | Alan George | Loyce Adams |
| Michael Heath | Eugene Wachspress | Randall LeVeque |
| Alex Pothen | Steve Serbin | James Ortega |
| Charles Romine | Larry Bales | Michael Saunders |
| | | Gene Golub |
| | | Linda Hayes |
| | | David Kincaid |

Of the University of Tennessee people, David worked most directly with Dr. Wachspress whom he has known for many years and whose research on iterative methods has had a strong impact on his own work. Dr. Wachspress and one of David's students (Vona) carried out a research study on new preconditioners for iterative methods. This work will be published soon.

David has been carrying on joint research with Adams and LeVeque on parallel methods for solving partial differential equations. The visits of Adams and LeVeque to ORNL provided an opportunity to continue this work and also to work on the completion of a joint paper which will appear soon.

Visits were arranged for Dr. Linda Hayes and Dr. David Kincaid who are colleagues of David's at The University of Texas and who are collaborators on joint grant-supported research projects. Their visits materially aided these projects.

One aspect of the program was the participation of visiting graduate students. Two students from Texas, Bi Roubolo Vona and Sheng-you Xiao, participated in this program. A report prepared by Mr. Xiao is appended to this report.

Because of the delay in clearance procedures, only one of the two students (Vona) was able to obtain access to Oak Ridge. This hampered the work to some extent. However, each student was able to access the Oak Ridge Computers from terminals located at The University of Tennessee. Moreover, the short course on parallel computers and many of the seminars were held at the University.

As indicated above, one of the main purposes of the visit was to learn about parallel machines and how to use them. This objective was accomplished to a considerable degree. After attending the short course on parallel computers David and his students were able to develop some rudimentary programs for use in their research. Moreover, they continue to have access to the Oak Ridge machines, as well as to other parallel machines, via telecommunications from The University of Texas.

At the algorithmic level, a great deal of information and many ideas were obtained as a result of interactions with staff members at ORNL and faculty at UTK as well as visitors. Attendance at the Conferences, Workshops, and Seminars was also most valuable.

The primary area of research which was developed relates to the spectral decomposition of iterative methods for solving large sparse linear systems arising from partial differential equations. These methods are in some sense similar to multigrid methods in that they focus on separate attacks on several parts of the eigenvalue spectrum of the iteration operator. The spectral decomposition scheme attempts to remove on dependence of several individual meshes, as required for multigrid methods, with the expectation that greater parallelism will result.

The research which was undertaken at Tennessee will be continued and expanded at Texas. It is anticipated that several publications will result.

B Seminar Notices

NUMERICAL LINEAR ALGEBRA SEMINAR¹

Cartesian grid methods for compressible flow in irregular regions

Randy Leveque

Departments of Mathematics and Applied Mathematics
University of Washington, Seattle

Date: September 16, 1987
Time: 3:00
Place: Tower 1 Conference Room
Building 9207, Y-12 Plant

ABSTRACT. An explicit finite volume method will be described that can be applied with arbitrary time steps on irregular grids in two dimensions. One dimensional normal and tangential Riemann problems are solved at cell interfaces and the resulting waves propagated over the grid. Far field and solid wall boundary conditions are easily implemented for the Euler equations. High resolution corrections can be made to obtain second order accuracy and sharp discontinuities.

One possible application is to Cartesian grids cut by irregular boundaries. This results in boundary cells that may be orders of magnitude smaller than the interior cells. The present approach allows one to use a time step appropriate for the regular cells with no stability restriction.

Entrance to Y-12 requires a pass. Contact Mitzy Denson (615) 574-3125 to obtain one.

¹This seminar is part of the Special Year on Numerical Linear Algebra sponsored by the UTK Departments of Computer Science and Mathematics, and the ORNL Mathematical Sciences Section, Engineering Physics and Mathematics Division.

NUMERICAL LINEAR ALGEBRA SEMINAR¹

Maintaining the Rank of Sparse LU Factors

Michael Saunders

Department of Operations Research
Stanford University

Date: October 26, 1987
Time: 4:00
Place: Small Conference Room, 1st Floor, Room 17
Bldg. 9207, Y-12 Plant

ABSTRACT. LUSOL is a package for computing LU factors of a general sparse matrix A, and for updating L and U when the rows or columns of A are altered.

When A is singular, L has full rank but U is singular. In order to estimate the rank of A it is necessary to keep U in trapezoidal form. We discuss some recent changes to LUSOL aimed at maintaining the trapezoidal form.

Entrance to Y-12 requires a pass. Contact Mitzy Denson (615) 574-3125 to obtain one.

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NUMERICAL LINEAR ALGEBRA SEMINAR¹

On the Complexity of Sparse LU and QR Factorization of Finite Element Matrices

Alan George, UT/ORNL Distinguished Scientist

Date: November 2, 1987
Time: 4:20
Place: Room 316, Ayres Hall
University of Tennessee

(Refreshments at 4:00 p.m. in Room 119, Ayres Hall)

ABSTRACT. Let A be an $n \times n$ sparse nonsingular matrix derived from a two-dimensional finite element mesh. If the matrix is symmetric and positive definite, and a nested dissection ordering is used, then the Cholesky factorization of A can be computed using $O(n^{3/2})$ arithmetic operations, and the number of nonzeros in the Cholesky factor is $O(n \log n)$. In this talk it is shown that the same complexity bounds can be attained when A is nonsymmetric and indefinite, and either Gaussian elimination with partial pivoting or orthogonal factorization is applied. Numerical experiments for a sequence of irregular mesh problems are provided.

¹This seminar is part of the Special Year on Numerical Linear Algebra sponsored by the UTK Departments of Computer Science and Mathematics, and the ORNL Mathematical Sciences Section, Engineering Physics and Mathematics Division.

NUMERICAL LINEAR ALGEBRA SEMINAR¹

The Theory of Moments in Linear Algebra

Gene Golub

Department of Computer Science
Stanford University

Date: November 9, 1987
Time: 4:00
Place: Small Conference Room, 1st Floor, Room 17
Bldg. 9207, Y-12 Plant

ABSTRACT. The Chebyshev semi-iterative method and Richardson method are classical techniques for solving large sparse linear systems of equations. Both methods, however, require the estimation of the extreme eigenvalues of the error operator. We describe these methods and relate them to the conjugate gradient method. We shall then demonstrate how modified moments can be used for estimating the required eigenvalues and for determining upper and lower bounds for the error in a particular norm.

Entrance to Y-12 requires a pass. Contact Mitzy Denson (615) 574-3125 to obtain one.

¹This seminar is part of the Special Year on Numerical Linear Algebra sponsored by the UTK Departments of Computer Science and Mathematics, and the ORNL Mathematical Sciences Section, Engineering Physics and Mathematics Division.

NUMERICAL LINEAR ALGEBRA SEMINAR¹

Parallel Solution of Triangular Systems on Distributed-Memory Multiprocessors

Michael T. Heath

Mathematical Sciences Section
Oak Ridge National Laboratory
Oak Ridge, Tennessee 37831

Date: November 16, 1987
Time: 4:20
Place: Room 316, Ayres Hall
University of Tennessee

(Refreshments at 4:00 p.m. in Room 119, Ayres Hall)

ABSTRACT. The solution of triangular systems of linear equations on conventional serial computers is usually considered an essentially trivial computation compared to matrix factorization. On parallel computers, especially those with distributed memory, the necessary communication among processors causes the relative costs of matrix factorization and triangular solution to be quite different from the serial case, with good efficiency being much more difficult to attain for triangular solution. We present several parallel algorithms for solving triangular systems partitioned by rows or by columns on distributed-memory multiprocessors. Performance of the algorithms is analyzed theoretically and compared both theoretically and empirically using implementations on commercial hypercubes.

¹This seminar is part of the Special Year on Numerical Linear Algebra sponsored by the UTK Departments of Computer Science and Mathematics, and the ORNL Mathematical Sciences Section, Engineering Physics and Mathematics Division.

NUMERICAL LINEAR ALGEBRA SEMINAR¹

Iterative Solution of Partial Differential Equations with Vector and Parallel Computers

David M. Young

Mathematics Department
University of Tennessee
and

Mathematical Sciences Section
Oak Ridge National Laboratory
on leave from

Departments of Mathematics and Computer Science
University of Texas at Austin

Date: November 23, 1987
Time: 4:20 p.m.
Place: Room 316, Ayres Hall
University of Tennessee

(Refreshments at 3:45 p.m. in Room 119, Ayres Hall)

ABSTRACT. A number of techniques, based on iterative methods, are described for solving large, sparse systems of linear algebraic equations arising from partial differential equations, with emphasis on the use of vector and parallel computers. Among the techniques considered are reordering techniques, multilevel techniques, polynomial preconditioning and related techniques, block methods and domain decomposition, multigrid and related techniques, and spectral decomposition methods.

¹This seminar is part of the Special Year on Numerical Linear Algebra sponsored by the UTK Departments of Computer Science and Mathematics, and the ORNL Mathematical Sciences Section, Engineering Physics and Mathematics Division.

NUMERICAL LINEAR ALGEBRA SEMINAR¹

Computing a Shortest Elimination Tree

Alex Pothen

Mathematical Sciences Section, ORNL
and

Department of Mathematics, UT
on leave from

Computer Science Department, Penn State

Date: December 7, 1987
Time: 4:20 p.m.
Place: Room 316, Ayres Hall
University of Tennessee

(Refreshments at 3:45 p.m. in Room 119, Ayres Hall)

ABSTRACT. The problem addressed in this talk arises in a graph model of Gaussian elimination of a symmetric, sparse matrix on a parallel computer. The *elimination tree* is a tree computable from the graph that models the parallelism in the elimination. The height of the tree is a measure of the parallel time required by Gaussian elimination.

We design an algorithm to compute a shortest elimination tree of a chordal graph. (A chordal graph is obtained when the vertices of a graph are ordered to reduce the number of new edges created during the elimination.) This algorithm requires time linear in the number of edges, and has several pleasing features: e.g., the new elimination tree as well as several data structures required in subsequent stages of the elimination are available as byproducts at the termination of the algorithm.

¹This seminar is part of the Special Year on Numerical Linear Algebra sponsored by the UTK Departments of Computer Science and Mathematics, and the ORNL Mathematical Sciences Section, Engineering Physics and Mathematics Division.

NUMERICAL LINEAR ALGEBRA SEMINAR¹

"A Survey of Element-by-Element Techniques for Finite Element Calculations"

Dr. Linda J. Hayes

Department of Aerospace Engineering
and Engineering Mechanics
The University of Texas

Date: Wednesday, December 9, 1987
Time: 3:30 p.m.
Place: Room 316, Ayres Hall
University of Tennessee

(Refreshments at 3:00 p.m. in Room 119, Ayres Hall)

ABSTRACT. In element-by-element techniques, finite element calculations are done using a data structure which accesses information one element at a time. This type of computation is very amenable to vector and parallel processing. This talk will be a survey of recent developments using element-by-element structures. It will include adaptive grid techniques and iterative methods. It will survey work done by G.R. Carey, L.J. Hayes, T.R. Hughes, and J.T. Oden.

¹This seminar is part of the Special Year on Numerical Linear Algebra sponsored by the UTK Departments of Computer Science and Mathematics, and the ORNL Mathematical Sciences Section, Engineering Physics and Mathematics Division.

NUMERICAL LINEAR ALGEBRA SEMINAR¹

Software & Numerical Experiments for Nonsymmetric Preconditioned Conjugate Gradient Methods

David R. Kincaid

The University of Texas at Austin

Date: Monday, December 14, 1987
Time: 2:00 p.m.
Place: Room 17 (Small Conference Room)
Building 9207, Y-12 Plant
Oak Ridge National Laboratory

ABSTRACT. A computer package NSPCG (for Nonsymmetric Preconditioned Conjugate Gradient) for solving large sparse linear systems by various iterative methods is presented. (NSPCG User's Guide, by Thomas C. Oppe, Wayne D. Joubert, and David R. Kincaid, Report CNA-216, November 1987, Center for Numerical Analysis, The University of Texas at Austin.) It contains a wide selection of preconditioners and accelerators for both symmetric and nonsymmetric coefficient matrices. In addition, several sparse matrix data structures are available for representing either structured or unstructured systems. NSPCG is a research-oriented computer package developed as part of the ITPACK Project of the Center for Numerical Analysis at The University of Texas at Austin.

¹This seminar is part of the Special Year on Numerical Linear Algebra sponsored by the UTK Departments of Computer Science and Mathematics, and the ORNL Mathematical Sciences Section, Engineering Physics and Mathematics Division.

NUMERICAL LINEAR ALGEBRA SEMINAR¹

Sparse Gaussian Elimination in Essential Time

Tim Peierls

Department of Computer Science
Cornell University

Date: January 25, 1988
Time: 10:00 a.m.
Place: Small Conference Room
Building 9207, Y-12
Oak Ridge National Laboratory

ABSTRACT. I present several (sequential) algorithms for Gaussian elimination that run in time proportional to the number of essential operations, that is, the number of floating point operations involving two structurally nonzero values. Other sparse linear equations solvers do not have this property, although they are tuned to be efficient for most real world problems. Although this work was motivated by the theoretical existence question and developed with the help of some graph theory, at least one of the resulting algorithms is quite efficient in practice.

Call Mitzy Denson at ORNL, 574-3125, if you should need a pass to get into the Laboratory.

¹This seminar is part of the Special Year on Numerical Linear Algebra sponsored by the UTK Departments of Computer Science and Mathematics, and the ORNL Mathematical Sciences Section, Engineering Physics and Mathematics Division.

NUMERICAL LINEAR ALGEBRA SEMINAR¹

"Parallel QR Factorization on a Hypercube Multiprocessor"

Eleanor Chu

Department of Mathematics
University of Tennessee

Date: February 1, 1988
Time: 4:00 p.m.
Place: Room 209A, Ayres Hall
University of Tennessee

(Refreshments at 3:30 p.m. in Room 119, Ayres Hall)

ABSTRACT. In this talk we present a new algorithm for computing the QR factorization of a rectangular matrix on a hypercube multiprocessor. The scheme involves the embedding of a two-dimensional grid in the hypercube network. We employ a global communication scheme which uses redundant computation to maintain data proximity, and the mapping strategy is such that for a fixed number of processors the processor idle time is small and either constant or grows linearly with the dimension of the matrix. A complexity analysis tells us what the aspect ratio of the embedded grid should be in terms of the shape of the matrix and the relative speeds of communication and computation. We shall report numerical experiments performed on an Intel Hypercube multiprocessor which support the theoretical results.

¹This seminar is part of the Special Year on Numerical Linear Algebra sponsored by the UTK Departments of Computer Science and Mathematics, and the ORNL Mathematical Sciences Section, Engineering Physics and Mathematics Division.

NUMERICAL LINEAR ALGEBRA SEMINAR¹

*"Stability Analysis of the Method of
Seminormal Equations for Linear Least Squares Problems"*

Åke Björck

Department of Mathematics
Linköping University
S-581 83 Linköping, Sweden

Date: February 8, 1988
Time: 4:00 p.m.
Place: Room 209A, Ayres Hall

(Refreshments at 3:30 p.m. in Room 119, Ayres Hall)

ABSTRACT. Consider the linear least squares problem $\min_x \|Ax - b\|_2$. When A is large and sparse, then often only the R -factor in the QR factorization of A is known. The solution x can then be computed from the seminormal equations $R^T R x = A^T b$. For this method the error in x is shown to be of the same order as for the method of normal equations. We show that by adding a correction step using only single precision we get a method which under mild conditions is as accurate as the QR method. The application of this method to the updating of a sparse R -factor of A when appending a column is discussed.

¹This seminar is part of the Special Year on Numerical Linear Algebra sponsored by the UTK Departments of Computer Science and Mathematics, and the ORNL Mathematical Sciences Section, Engineering Physics and Mathematics Division.

JOINT
UTK DEPARTMENT OF STATISTICS COLLOQUIUM
AND
NUMERICAL LINEAR ALGEBRA SEMINAR¹

"Sparse Matrix Computations in Analysis of Variance"

George Ostrouchov

Mathematical Sciences Section
Oak Ridge National Laboratory
Oak Ridge, TN 37831

Date: February 25, 1988 (Thursday)
Time: 12:15 - 1:15 p.m.
Place: Room 51, Glocker Bus. Admin.
University of Tennessee, Knoxville**

¹

ABSTRACT. Unbalanced data in Analysis of Variance require the explicit solution of a least squares problem. The least squares problem is sparse and can be very large, thus its solution can benefit from the use of sparse matrix techniques. The use of standard sparse matrix techniques in combination with symbolic processing that takes advantage of the special matrix structure can produce a very efficient direct method. This talk will briefly describe the analysis of variance problem and standard sparse matrix techniques for the direct solution of least squares problems. Most of the talk will concentrate on the application of sparse matrix techniques to the analysis of variance problem and symbolic processing based on model term index sets.

¹This seminar is part of the Special Year on Numerical Linear Algebra sponsored by the UTK Departments of Computer Science and Mathematics, and the ORNL Mathematical Sciences Section, Engineering Physics and Mathematics Division.

¹Public parking is available at the University Center Parking Garage on the corner of Stadium Drive (opposite 15th Street at West Cumberland Avenue) and Andy Holt Avenue.

NUMERICAL LINEAR ALGEBRA SEMINAR¹

"Some Ideas in the Solution of Sparse Linear Least Squares Problems"

Esmond Ng

Mathematical Sciences Section
Oak Ridge National Laboratory
Oak Ridge, TN 37831

Date: February 29, 1988
Time: 4:00 p.m.
Place: Room 209A, Ayres Hall
University of Tennessee, Knoxville

(Refreshments at 3:30 p.m. in Room 119, Ayres Hall)

ABSTRACT. The problem of solving large sparse linear least squares problems is considered. The solution method is based on orthogonal factorizations. The data structures and an algorithm for computing the orthogonal decomposition will be presented. An attractive feature of the approach is that both the orthogonal transformations and the triangular factor are saved. Hence multiple least squares problems which have the same coefficient matrix but different right hand sides can be solved very efficiently. Techniques for handling rank-deficient problems will be described.

¹This seminar is part of the Special Year on Numerical Linear Algebra sponsored by the UTK Departments of Computer Science and Mathematics, and the ORNL Mathematical Sciences Section, Engineering Physics and Mathematics Division.

NUMERICAL LINEAR ALGEBRA SEMINAR¹

"Truncated SVD Solutions to Ill-posed Problems With Ill-determined Numerical Rank"

Per Christian Hansen

Copenhagen University Observatory
Øster Voldgade 3, DK-1350
København K, Denmark

Date: March 7, 1988
Time: 4:00 p.m.
Place: Room 209A, Ayres Hall
University of Tennessee

(Refreshments at 3:30 p.m. in Room 119, Ayres Hall)

ABSTRACT. Fredholm integral equations of the first kind lead to algebraic least squares problems with ill-conditioned matrices having an ill-determined numerical rank. These problems can be solved by means of the *truncated SVD* (TSVD) method.

We show that if a solution exists to the *unperturbed* integral equation, then the TSVD solution is insensitive to perturbations of the right-hand side provided that the truncation parameter is chosen properly. We also show that under this assumption, the TSVD solution is guaranteed to be close to the solution obtained by regularization in standard form, and both solutions are close to the solution to the unperturbed problem and they are *reasonable* in the sense of Varah's definition.

Hence, since the SVD always gives *insight* into the problem, TSVD is a favorable alternative to standard-form regularization for solving ill-posed problems, *independently* of the existence of a gap in the singular value spectrum.

¹This seminar is part of the Special Year on Numerical Linear Algebra sponsored by the UTK Departments of Computer Science and Mathematics, and the ORNL Mathematical Sciences Section, Engineering Physics and Mathematics Division.

NUMERICAL LINEAR ALGEBRA SEMINAR¹

"A Toolbox for Very Special Eigenvalue Problems"

Ralph Byers

Department of Mathematics
University of Kansas
Lawrence, KS 66045

Date: March 14, 1988
Time: 10:00 a.m.
Place: Small Conference Room
Room 9207, Y-12
Oak Ridge National Laboratory

ABSTRACT. A matrix has a very special structure, if it has two kinds of structure, e.g., Hermitian and Hamiltonian or complex symmetric and symplectic. Each very special structure imparts a very special structure to the eigenvalues and eigenvectors. The toolbox contains special similarity transformations, condensed forms, shifts of origin, and common subproblems for algorithms for a variety of eigenvalue problems with very special structure. A proper selection of tools gives a *QR*-like or a Jacobi-like numerical method for calculating eigenvalues and eigenvectors. These structure preserving algorithms are more efficient and numerically stable than conventional methods. Often they produce the eigenvalues and eigenvectors of a nearby matrix with very special structure.

¹This seminar is part of the Special Year on Numerical Linear Algebra sponsored by the UTK Departments of Computer Science and Mathematics, and the ORNL Mathematical Sciences Section, Engineering Physics and Mathematics Division.

NUMERICAL LINEAR ALGEBRA SEMINAR¹

"Iterative Solution of Sylvester's Equation"

Eugene Wachspress

Department of Mathematics
University of Tennessee

Date: March 21, 1988
Time: 10:00 a.m.
Place: Small Conference Room
Room 9207, Y-12
Oak Ridge National Laboratory

ABSTRACT. Most of the computation time in numerical solution of a Sylvester equation of order n is spent on the $O(n^3)$ reduction of matrices of order n from tridiagonal (Hessenberg for the non-symmetric case) to diagonal (Schur) form. This reduction can be replaced by an $O(n^2)$ iteration. The theoretical foundations for this iteration were developed for solution of elliptic PDE's by Alternating Direction Implicit (ADI) iteration. Application of the ADI theory to Sylvester's equation will be described. The ADI iteration is better suited for this application than for the problems for which it was initially devised. A restrictive matrix commutation condition required for the PDE iteration is not needed for the Sylvester iteration.

¹This seminar is part of the Special Year on Numerical Linear Algebra sponsored by the UTK Departments of Computer Science and Mathematics, and the ORNL Mathematical Sciences Section, Engineering Physics and Mathematics Division.

NUMERICAL LINEAR ALGEBRA SEMINAR¹

"Robust Statistics Computations on Parallel Computing Machines"

Virginia Klema

Laboratory for Information and Decision Systems
Massachusetts Institute of Technology
Cambridge, MA 02139

Date: March 28, 1988
Time: 4:00 – 5:00 p.m.
Place: Room 209A, Ayres Hall
University of Tennessee

(Refreshments at 3:30 p.m. in Room 119, Ayres Hall)

ABSTRACT. Many of the computations for robust statistics are parallel-certain in the sense that much of the work can be done on different processors at the same time. Reporting of the final results can be deferred, and there is no necessity for processor to processor communication. Jack-knife, bootstrap, and iteratively reweighted least squares are such computationally intensive applications.

Computational results will be reported from the BBN Butterfly and the Intel hypercube for the Jack-knife. These two machines have apparently different communication mechanisms; however, we will demonstrate that similar partitioning strategies must be used to achieve a balanced load of work on multiple processors.

¹This seminar is part of the Special Year on Numerical Linear Algebra sponsored by the UTK Departments of Computer Science and Mathematics, and the ORNL Mathematical Sciences Section, Engineering Physics and Mathematics Division.

NUMERICAL LINEAR ALGEBRA SEMINAR¹

"Finding Eigenvalues and Eigenvectors of Unsymmetric Matrices Using a Distributed-memory Multiprocessor"

G. A. Geist

Mathematical Sciences Section
Oak Ridge National Laboratory

Date: April 11, 1988
Time: 4:00 – 5:00 p.m.
Place: Room 209A, Ayres Hall
University of Tennessee

(Refreshments at 3:30 p.m. in Room 119, Ayres Hall)

ABSTRACT. The best known method for finding the eigenvalues of dense unsymmetric matrices is the implicit double shift QR iteration. The complexity and large volume of communication required in this algorithm have hindered distributed-memory implementations. We will discuss several parallel implementations of this algorithm and their performance on the Intel iPSC.

Recent advances in distributed-memory triangular solutions have been used to develop an algorithm for finding the eigenvectors of the matrix. While Amdahl's Law limits our present implementations of the QR iteration to a speedup of about 10, the performance of the eigenvector routines does not suffer from the same limitation.

Research supported by the Applied Mathematical Sciences Research Program of the Office of Energy Research, U.S. Department of Energy.

¹This seminar is part of the Special Year on Numerical Linear Algebra sponsored by the UTK Departments of Computer Science and Mathematics, and the ORNL Mathematical Sciences Section, Engineering Physics and Mathematics Division.

NUMERICAL LINEAR ALGEBRA SEMINAR¹

"Parallel Algorithms for Solving Systems of Nonlinear Equations on a Hypercube Computer"

Tom Coleman

Department of Computer Science
Cornell University
Ithaca, NY 14853

Date: April 18, 1988
Time: 10:00 a.m.
Place: Small Conference Room
Building 9207, Y-12
Oak Ridge National Laboratory

ABSTRACT. We discuss the development of parallel algorithms for the solution of systems of nonlinear equations on a hypercube computer. Specifically, for the square case we propose distributed rank-1 secant and finite-difference Newton methods as well as a new parallel multi-secant method. All methods discussed exhibit strong global convergence properties and at least local superlinear convergence. For the rectangular case, we discuss parallel variants of the Minpack procedures (including new parallel QR-factorization techniques).

In this talk we will emphasize implementation ideas and numerical results obtained on the Cornell Theory Center's Intel iPSC.

Entrance to Y-12 requires a pass. Call Mitzy Denson at 574-3125 (ORNL) to obtain one.

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NUMERICAL LINEAR ALGEBRA SEMINAR¹

"On the Convergence Analysis of Algorithms for Constrained Optimization"

Tom Coleman

Department of Computer Science
Cornell University
Ithaca, NY 14853

Date: April 19, 1988
Time: 4:00 – 5:00 p.m.
Place: Room 209A, Ayres Hall
University of Tennessee

(Refreshments at 3:30 p.m. in Room 119, Ayres Hall)

ABSTRACT. In this talk we propose and develop techniques for analyzing the local convergence behaviour of algorithms for constrained optimization. We will illustrate the utility of these techniques by considering various algorithms (new and old) and establishing their superlinearity. The focus of attention in this development is the matrix representing the Jacobian of a related (but not computable) nonlinear system.

¹This seminar is part of the Special Year on Numerical Linear Algebra sponsored by the UTK Departments of Computer Science and Mathematics, and the ORNL Mathematical Sciences Section, Engineering Physics and Mathematics Division.

NUMERICAL LINEAR ALGEBRA SEMINAR¹

"Exploiting Sparsity in Large-Scale Optimization"

Tom Coleman

Department of Computer Science
Cornell University
Ithaca, NY 14853

Date: April 20, 1988
Time: 10:00 a.m.
Place: Small Conference Room
Building 9207, Y-12
Oak Ridge National Laboratory

ABSTRACT. We will review recent progress in the finite-difference approach to large sparse optimization problems. Theory, algorithms, and software will be discussed with emphasis on practicalities. We will conclude with some thoughts on the potential for parallel computation.

Entrance to Y-12 requires a pass. Call Mitzy Denson (ORNL) (615) 574-3125 to obtain one.

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NUMERICAL LINEAR ALGEBRA SEMINAR¹

"Error-free Sparse Least Squares"

Sallie Keller-McNulty

Department of Statistics
Kansas State University
Manhattan, KS 66506

Date: May 9, 1988
Time: 4:00 – 5:00 p.m.
Place: Room 309A, Ayres Hall
University of Tennessee

(Refreshments at 3:30 p.m. in Room 119, Ayres Hall)

ABSTRACT. Numerical methods which allow error-free computations of sparse matrix decomposition and least squares solutions are developed. These methods require that the sparse linear systems of equations have rational entries. To avoid error that is inherent in floating-points arithmetic, multiple modulus residue arithmetic is applied to a modified version of the LDU factorization.

¹This seminar is part of the Special Year on Numerical Linear Algebra sponsored by the UTK Departments of Computer Science and Mathematics, and the ORNL Mathematical Sciences Section, Engineering Physics and Mathematics Division.

NUMERICAL LINEAR ALGEBRA SEMINAR¹

"Parallel Least Squares Algorithms in Signal Processing"

Robert J. Plemmons

Departments of Computer Science and Mathematics
North Carolina State University
Raleigh, NC 27695-8205

Date: May 16, 1988
Time: 10:00 a.m.
Place: Small Conference Room
Building 9207, Y-12
Oak Ridge National Laboratory

ABSTRACT. We are concerned with the investigation of parallel algorithms for least squares modifications in signal processing. The first part of the talk involves a comparison of various algorithms for least squares updating and downdating on the hypercube, including comparisons of Givens rotations and Householder transformations for multiple updates. Computational tests on an iPSC64 hypercube are discussed. This part includes joint work with D. Agrawal, C. Henkel, and S. Kim at NCSU and with M. Heath at ORNL.

The second part of the talk involves parallel least squares modifications using inverse factorizations. The process of modifying least squares computations by updating the covariance matrix has been used in control and signal processing for some time in the context of linear sequential filtering. Here we give an alternative derivation of the process and provide extensions to downdating. Our purpose is to develop algorithms that are amenable to implementation on modern multiprocessor architectures. We have attempted to provide some new insights into least squares modification processes and to suggest parallel algorithms for implementing Kalman type sequential filters in the analysis and solution of estimation problems in control and signal processing. This part of the presentation is joint with C.-T. Pan at NIU.

Entrance to Y-12 requires a pass. Contact Mitzy Denson (615) 574-3125 to obtain one.

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NUMERICAL LINEAR ALGEBRA SEMINAR¹

"On An Eigenreduction Algorithm for Definite Matrix Pairs"

Krešimir Veselić

Fernuniversität
Hagen, Germany

Date: Thursday, May 19, 1988
Time: 9:00 – 10:15 a.m.
Place: Room 209A, Ayres Hall
University of Tennessee

ABSTRACT. In applications symmetric matrix pairs A, B occur, where neither A , nor B is positive definite but an (unknown) linear combination $A - \mu B$ is. The proposed algorithm is designed to solve the problem $Ax = \lambda Bx$ for such pairs. Although the algorithm is of the Jacobi type, it seems to be competitive with the related QR-algorithms.

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NUMERICAL LINEAR ALGEBRA SEMINAR¹

"Algorithms for Equality Constrained Least Squares Problems"

Jesse L. Barlow

Computer Science Department
The Pennsylvania State University
University Park, PA 16802

Date: June 6, 1988
Time: 4:00 - 5:00 p.m.
Place: Room 309A, Ayres Hall
University of Tennessee

(Refreshments at 3:30 p.m. in Room 119, Ayres Hall)

ABSTRACT. We consider two direct methods for solving equality constrained least squares problems where both the constraint matrix and the least squares matrix are large and sparse. The first method discussed is the direct factorization of a weighted matrix and the second is the deferred correction scheme proposed by Van Loan. For either of these schemes to be stable, the rank of the constraint matrix must be accurately detected. We examine the sparsity and stability of three different rank detection procedures.

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NUMERICAL LINEAR ALGEBRA SEMINAR¹

"Some Practical Aspects of Elimination Trees in Sparse Factorization"

Joseph W. H. Liu

Department of Computer Science
York University
Downsview, Ontario, Canada M3J 1P3

Date: Monday, June 13, 1988
Time: 10:00-11:00 a.m.
Place: Small Conference Room
Building 9207, Y-12
Oak Ridge National Laboratory

ABSTRACT. The elimination tree has emerged as an important structure in the study of direct solution of large sparse linear systems. It is useful in designing efficient solution methods for serial, vector and parallel machines. In this talk, we consider a number of properties of such elimination tree structure that are relevant to sparse factorization. For each property introduced, some practical applications are presented.

¹This seminar is part of the Special Year on Numerical Linear Algebra sponsored by the UTK Departments of Computer Science and Mathematics, and the ORNL Mathematical Sciences Section, Engineering Physics and Mathematics Division.

NUMERICAL LINEAR ALGEBRA SEMINAR¹

"Jacobi Algorithms for Eigenproblems on a Hypercube"

Haesun Park

Department of Computer Science
University of Minnesota
Minneapolis, MN 55455

Date: June 20, 1988
Time: 3:00 - 4:00 p.m.
Place: Small Conference Room
Building 9207, Y-12
Oak Ridge National Laboratory

ABSTRACT. The recently exploding interest in parallel computing has given rise to many new ways to implement Jacobi algorithms. We study five well known parallel orderings for implementing the method, and show that they are all equivalent to one another. In addition, we establish that these orderings are also equivalent to the classical cyclic-by-rows ordering and share the same convergence properties. Thus, we show that the various researchers came up with essentially the same idea independently and concurrently, and we prove convergence of their new methods.

We describe implementations of Jacobi algorithms with various orderings for solving eigenproblems on the NCUBE hypercube. We introduce two new orderings that require minimum number of stages per sweep with minimal message passing. A block-column scheme to handle the problems when the matrix size does not fit the number of available processors is described.

¹This seminar is part of the Special Year on Numerical Linear Algebra sponsored by the UTK Departments of Computer Science and Mathematics, and the ORNL Mathematical Sciences Section, Engineering Physics and Mathematics Division.

C Workshop Announcements

SHORT COURSE ON THE SOLUTION OF SPARSE SYSTEMS OF EQUATIONS

Numerical Linear Algebra Year:
The University of Tennessee
The Oak Ridge National Laboratory

October 5-9, 1987

The Departments of Computer Science and Mathematics of The University of Tennessee at Knoxville (UTK) and the Mathematical Sciences Section of the Oak Ridge National Laboratory (ORNL) have organized a *Numerical Linear Algebra Year* from September 1, 1987 to June 30, 1988. During this period, leading researchers in numerical linear algebra and related areas of scientific computation and computer science will visit the University and the Laboratory. The activities for the Year are being supported by the U.S. Air Force Office of Scientific Research, the U.S. Dept. of Energy, the National Security Agency, the National Science Foundation, and the Science Alliance, a state-supported program at the University of Tennessee.

As part of the NLA year activities, a short course on the solution of large sparse systems of linear equations will be held during the week of October 5, 1987 in Room 221 of the University Center on the UTK campus. Two 75 minute lectures will be given each morning (9:00-10:15, 10:45-noon), with an intervening coffee break. Informal afternoon sessions will be organized each day on the basis of requests from attendees who may wish either more elementary background material, or material that is more advanced than that given in the morning lectures.

The lecturers will be Dr. J. Alan George (UTK and ORNL), Dr. James M. Ortega (University of Virginia) and Dr. David M. Young (University of Texas at Austin). George will focus on direct methods, while Ortega and Young will deal with iterative methods. Introductory material will be discussed for both classes of methods, so that graduate students and non-experts should be able to benefit from the course. Algorithms for solving large sparse systems on parallel computers also will be discussed.

Those wishing to attend, or requiring further information, should contact Dr. Alan George at (615) 974-0995 (UTK) or Dr. Robert C. Ward at (615) 574-3125 (ORNL).

Schedule and Tentative Titles

Monday October 5

| | | |
|-------------|--------|--|
| 9:00-10:15 | George | Sparse Positive Definite Systems: Basic Material |
| 10:15-10:45 | | Coffee Break |
| 10:45-12:00 | Ortega | Parallel Architectures |
| 12:00 | | Lunch |
| 1:30-3:00 | | Informal Sessions |

Tuesday October 6

| | | |
|-------------|--------|--|
| 9:00-10:15 | George | Symbolic Factorization and Data Structures |
| 10:15-10:45 | | Coffee Break |
| 10:45-12:00 | Ortega | Jacobi and SOR Methods |
| 12:00 | | Lunch |
| 1:30-3:00 | | Informal Sessions |

Wednesday October 7

| | | |
|-------------|--------|---|
| 9:00-10:15 | George | Elimination Trees and Their Uses |
| 10:15-10:45 | | Coffee Break |
| 10:45-12:00 | Ortega | Preconditioned Conjugate Gradient Methods |
| 12:00 | | Lunch |
| 1:30-3:00 | | Informal Sessions |

Thursday October 8

| | | |
|-------------|--------|---|
| 9:00-10:15 | George | Algorithms for Shared-Memory Parallel Architectures |
| 10:15-10:45 | | Coffee Break |
| 10:45-12:00 | Young | Iterative Algorithms for the Symmetric Case |
| 12:00 | | Lunch |
| 1:30-3:00 | | Informal Sessions |

Friday October 9

| | | |
|-------------|--------|--|
| 9:00-10:15 | George | Algorithms for Local-Memory Parallel Architectures |
| 10:15-10:45 | | Coffee Break |
| 10:45-12:00 | Young | Iterative Algorithms for the Unsymmetric Case |
| 12:00 | | Lunch |
| 1:30-3:00 | | Informal Sessions |

A Short Course
on
EIGENVALUES AND SINGULAR VALUES

Numerical Linear Algebra Year:
The University of Tennessee
The Oak Ridge National Laboratory

January 11-15, 1988

The Departments of Computer Science and Mathematics of The University of Tennessee at Knoxville (UTK) and the Mathematical Sciences Section of the Oak Ridge National Laboratory (ORNL) have organized a *Numerical Linear Algebra Year* from September 1, 1987 to June 30, 1988. During this period, leading researchers in numerical linear algebra and related areas of scientific computation and computer science will visit the University and the Laboratory. The activities for the Year are being supported by the U.S. Air Force Office of Scientific Research, the U.S. Dept. of Energy, the National Security Agency, the National Science Foundation, and the Science Alliance, a state-supported program at the University of Tennessee.

As part of the NLA year activities, a short course on computational methods for finding eigenvalues and singular values of matrices will be held during the week of January 11, 1988 at the Best Western Campus Inn, Knoxville. Two 75 minute lectures will be given each morning (9:00-10:15, 10:45-noon), with an intervening coffee break. Informal afternoon sessions will be organized each day on the basis of requests from attendees who may wish either more elementary background material, or material that is more advanced than that given in the morning lectures.

The lecturers will be Professor Beresford Parlett (University of California, Berkeley), and Professor James Demmel (Courant Institute of Mathematical Sciences, New York). Parlett will focus on Krylov Subspace methods, which are particularly well-suited for very large sparse eigenvalue problems. Demmel will deal with more conventional methods based on the QR algorithm. Introductory material will be discussed for both classes of methods, so that graduate students and non-experts should be able to benefit from the course. The role of parallel computers in eigenvalue and singular value computations also will be discussed.

Those wishing to attend, or requiring further information, should contact Dr. Alan George at (615) 974-0995 (UTK) or Dr. Robert C. Ward at (615) 574-3125 (ORNL).

Schedule and Tentative Titles

| | | |
|-----------------------|----------|---|
| Monday, January 11 | | |
| 9:00-10:15 | Demmel | Theory and Algorithms for the Dense, Nonsymmetric Eigenproblem |
| 10:15-10:45 | | Coffee Break |
| 10:45-12:00 | Parlett | Various Eigenvalue Tasks, Error Estimates, Rayleigh-Ritz Approximations, Subspace Iteration, Lanczos, Arnoldi |
| 12:00 | | Lunch |
| 1:30-3:00 | | Informal Sessions |
| Tuesday, January 12 | | |
| 9:00-10:15 | Demmel | Theory and Algorithms for the Dense, Symmetric Eigenproblem |
| 10:15-10:45 | | Coffee Break |
| 10:45-12:00 | Parlett | Krylov Subspaces and Their Approximation Properties, Orthogonality Loss and Paige's Theorem |
| 12:00 | | Lunch |
| 1:30-3:00 | | Informal Sessions |
| Wednesday, January 13 | | |
| 9:00-10:15 | Demmel | Condition Numbers and Error Bounds for Eigenvalues and Eigenvectors |
| 10:15-10:45 | | Coffee Break |
| 10:45-12:00 | Parlett | Implementation Options, Stopping Criteria, Infinite Eigenvalues |
| 12:00 | | Lunch |
| 1:30-3:00 | | Informal Sessions |
| Thursday, January 14 | | |
| 9:00-10:15 | Demmel | A Guided Tour of EISPACK |
| 10:15-10:45 | | Coffee Break |
| 10:45-12:00 | Parlett | The Nonsymmetric Case, Residual Error Bounds |
| 12:00 | | Lunch |
| 1:30-3:00 | | Informal Sessions |
| Friday, January 15 | | |
| 9:00-10:15 | Demmel | Recent Research in Parallel Algorithms for the Eigenproblem |
| 10:15-10:45 | | Coffee Break |
| 10:45-12:00 | Sorenson | To be announced |
| 12:00 | | Lunch |
| 1:30-3:00 | | Informal Sessions |

A Short Course
on
NUMERICAL SOLUTION OF
LEAST SQUARES PROBLEMS

Numerical Linear Algebra Year:

The University of Tennessee
The Oak Ridge National Laboratory
May 2-6, 1988

The Departments of Computer Science and Mathematics of The University of Tennessee at Knoxville (UTK) and the Mathematical Sciences Section of the Oak Ridge National Laboratory (ORNL) have organized a *Numerical Linear Algebra Year* from September 1, 1987 to June 30, 1988. During this period, leading researchers in numerical linear algebra and related areas of scientific computation and computer science will visit the University and the Laboratory. The activities for the Year are being supported by the U.S. Air Force Office of Scientific Research, the U.S. Dept. of Energy, the National Security Agency, the National Science Foundation, and the Science Alliance, a state-supported program at the University of Tennessee.

As part of the NLA year activities, a short course on Numerical Methods for Least Squares Problems will be held during the week of May 2-6, 1988, at the Holiday Inn at Cedar Bluff. Two 75 minute lectures will be given each morning (9:00-10:15, 10:45-noon), with an intervening coffee break. Informal afternoon sessions will be organized each day on the basis of requests from attendees who may wish either more elementary background material, or material that is more advanced than that given in the morning lectures.

The lecturers will be Prof. Robert J. Plemmons (North Carolina State University), Dr. Michael T. Heath (ORNL), Dr. George Ostrouchov (ORNL), and Dr. Esmond Ng (ORNL). Plemmons will focus on the basic mathematical theory and standard techniques for least squares problems, followed by discussions on parallel algorithms and applications. Heath will focus his lectures on methods for dealing with large sparse least squares problems, Ostrouchov will discuss sparse matrix techniques designed for statistical applications, and Ng will describe the design and implementation of a software package for solving large sparse least squares problems. Introductory material will be discussed, so that graduate students and non-experts should be able to benefit from the course.

Those wishing to attend, or requiring further information, should contact Dr. Alan George at (615) 974-0995 (UTK) or Dr. Robert C. Ward at (615) 574-3125 (ORNL).

Schedule and Tentative Titles

Monday, May 2

| | | |
|-------------|----------|--|
| 9:00-10:15 | Plemmons | "Mathematical Properties" |
| 10:15-10:45 | | Coffee Break |
| 10:45-12:00 | Heath | "A Structural Approach to Sparse Least Squares Computations" |
| 12:00-1:30 | | Lunch |
| 1:30-3:00 | | Informal Sessions |

Tuesday, May 3

| | | |
|-------------|----------|---|
| 9:00-10:15 | Plemmons | "Numerical Methods" |
| 10:15-10:45 | | Coffee Break |
| 10:45-12:00 | Heath | "Variations and Extensions of the Structural Approach to Sparse Least Squares Computations" |
| 12:00-1:30 | | Lunch |
| 1:30-3:00 | | Informal Sessions |

Wednesday, May 4

| | | |
|-------------|----------|---|
| 9:00-10:15 | Plemmons | "Constrained Problems and Modified Problems " |
| 10:15-10:45 | | Coffee Break |
| 10:45-12:00 | Heath | "A Survey of Other Methods for Sparse Least Squares Computations" |
| 12:00-1:30 | | Lunch |
| 1:30-3:00 | | Informal Sessions |

Thursday, May 5

| | | |
|-------------|------------|---|
| 9:00-10:15 | Plemmons | "Parallel Algorithms " |
| 10:15-10:45 | | Coffee Break |
| 10:45-12:00 | Ostrouchov | "Sparse Least Squares Computations in Statistical Applications" |
| 12:00-1:30 | | Lunch |
| 1:30-3:00 | | Informal Sessions |

Friday, May 6

| | | |
|-------------|----------|---|
| 9:00-10:15 | Plemmons | "Some Applications, Including Signal Processing " |
| 10:15-10:45 | | Coffee Break |
| 10:45-12:00 | Ng | "Software for Sparse Least Squares Computations" |
| 12:00-1:30 | | Lunch |
| 1:30-3:00 | | Informal Sessions |

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